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LOGINID: SSPTANXR1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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                     Welcome to STN International
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NEWS
         DEC 01
NEWS
                 ChemPort single article sales feature unavailable
NEWS
         FEB 02
                 Simultaneous left and right truncation (SLART) added
                 for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS
         FEB 02
                 GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS
         FEB 06
                 Patent sequence location (PSL) data added to USGENE
NEWS
         FEB 10
                 COMPENDEX reloaded and enhanced
NEWS
      7
         FEB 11
                 WTEXTILES reloaded and enhanced
NEWS
      8 FEB 19
                 New patent-examiner citations in 300,000 CA/CAplus
                 patent records provide insights into related prior
NEWS
      9
         FEB 19
                 Increase the precision of your patent queries -- use
                 terms from the IPC Thesaurus, Version 2009.01
NEWS 10
         FEB 23
                 Several formats for image display and print options
                 discontinued in USPATFULL and USPAT2
         FEB 23
                 MEDLINE now offers more precise author group fields
NEWS 11
                 and 2009 MeSH terms
                 TOXCENTER updates mirror those of MEDLINE - more
NEWS 12
         FEB 23
                 precise author group fields and 2009 MeSH terms
NEWS 13
         FEB 23
                 Three million new patent records blast AEROSPACE into
                 STN patent clusters
NEWS 14
         FEB 25
                 USGENE enhanced with patent family and legal status
                 display data from INPADOCDB
         MAR 06
                 INPADOCDB and INPAFAMDB enhanced with new display
NEWS 15
                 formats
NEWS 16
         MAR 11
                 EPFULL backfile enhanced with additional full-text
                 applications and grants
         MAR 11
NEWS 17
                 ESBIOBASE reloaded and enhanced
                 CAS databases on STN enhanced with new super role
NEWS 18
         MAR 20
                 for nanomaterial substances
                 CA/CAplus enhanced with more than 250,000 patent
NEWS 19
         MAR 23
                 equivalents from China
NEWS 20
         MAR 30
                 IMSPATENTS reloaded and enhanced
NEWS 21
         APR 03
                 CAS coverage of exemplified prophetic substances
                  enhanced
NEWS 22
         APR 07
                 STN is raising the limits on saved answers
NEWS 23
         APR 24
                 CA/CAplus now has more comprehensive patent assignee
                  information
                 USPATFULL and USPAT2 enhanced with patent
NEWS 24
         APR 26
                 assignment/reassignment information
NEWS 25
         APR 28
                 CAS patent authority coverage expanded
NEWS 26
         APR 28
                 ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 27
         APR 28
                 Limits doubled for structure searching in CAS
                 REGISTRY
NEWS 28 MAY 08
                 STN Express, Version 8.4, now available
NEWS 29
         MAY 11
                 STN on the Web enhanced
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- NEWS 30 MAY 11 BEILSTEIN substance information now available on STN Easy
- NEWS 31 MAY 14 DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
- NEWS 32 MAY 15 INPADOCDB and INPAFAMDB enhanced with Chinese legal status data

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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=> file reg
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SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

FULL ESTIMATED COST

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DICTIONARY FILE UPDATES: 20 MAY 2009 HIGHEST RN 1147939-89-6

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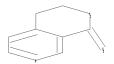
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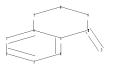
http://www.cas.org/support/stngen/stndoc/properties.html

=>

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chain nodes :



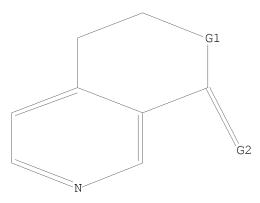
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11
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10
exact/norm bonds :
4-7 5-10 7-8 8-9 9-10 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:0, N
G2:0,S
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS
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STRUCTURE UPLOADED L1

=> d 11

L1 HAS NO ANSWERS

L1



G1 O, N

G2 O, S

Structure attributes must be viewed using STN Express query preparation.

=> s 11 full

FULL SEARCH INITIATED 19:49:21 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -84387 TO ITERATE

100.0% PROCESSED

84387 ITERATIONS

SEARCH TIME: 00.00.02

L2 384 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 185.88 186.10

384 ANSWERS

FULL ESTIMATED COST

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=> s 12 full L3 279 L2

=> file reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST ENTRY SESSION 1.00 187.10

SINCE FILE

TOTAL

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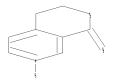
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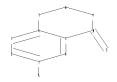
http://www.cas.org/support/stngen/stndoc/properties.html

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chain nodes :

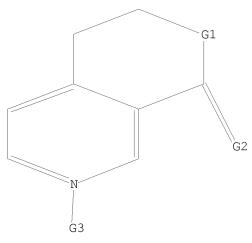


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ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
1-15 10-11
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 4-7 \quad 5-6 \quad 5-10 \quad 7-8 \quad 8-9 \quad 9-10
exact/norm bonds :
1-15 4-7 5-10 7-8 8-9 9-10 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:0,N
G2:0,S
G3:H,CH3
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 15:CLASS
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=> d 14

L4 HAS NO ANSWERS

L4 STR



G1 O, N

G2 0, S

G3 H, Me

Structure attributes must be viewed using STN Express query preparation.

76 ANSWERS

TOTAL

SINCE FILE

=> s 14 full

FULL SEARCH INITIATED 19:51:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 84387 TO ITERATE

100.0% PROCESSED 84387 ITERATIONS

SEARCH TIME: 00.00.02

L5 76 SEA SSS FUL L4

=> file caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST ENTRY SESSION 185.88 372.98

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FILE LAST UPDATED: 20 May 2009 (20090520/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009
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=> s 15 full L6 15 L5

=> d ibib abs hitstr tot

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ACCESSION NUMBER:
                              2008:1244945 CAPLUS
DOCUMENT NUMBER:
                              149:478670
TITLE:
                              A pharmaceutical compositions containing lactone type
                              pyridine derivatives as an effective ingredient for
                              the prevention and treatment of ischemia
INVENTOR(S):
                              Cho, Yong-Baik; Lee, Junwon; Yi, Jung Bum; Lee, Nam
                              Kyu; Lee, Bong-Yong; Hwang, Ki-Chul; Lim, Soyeon;
                              Chang, Woochul; Chung, Ji Hyung; Lee, Byung Ho; Seo,
                              SK Chemicals Co., Ltd., S. Korea
PATENT ASSIGNEE(S):
SOURCE:
                              PCT Int. Appl., 72pp.
                              CODEN: PIXXD2
DOCUMENT TYPE:
                              Patent
LANGUAGE:
                              English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
      PATENT NO.
                                                   APPLICATION NO.
                            KIND
                                      DATE
                                                                                DATE
                             ____
                                      _____
                                                    _____
                                                   WO 2008-KR2030
      WO 2008123756
                              A1
                                      20081016
                                                                               20080410
          W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ,
          W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, MI, MR, NE, SN, TD,
               TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
               TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,
               AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
                             Α
                                      20081015
                                                     KR 2007-35075
      KR 2008091949
                                                                                 20070410
                                                     KR 2007-35075
                                                                             A 20070410
PRIORITY APPLN. INFO.:
      The present invention relates to a pharmaceutical composition comprising a
      lactone type pyridine derivative for the prevention and treatment of ischemic
      diseases, more particularly to a pharmaceutical composition for preventing and
      treating ischemic diseases comprising a lactone type pyridine derivative or a
      pharmaceutically acceptable salt thereof as an active ingredient, which
     provides superior cell-protecting effect and calcium homeostasis and HSP
      (heat shock protein) expression controlling effect.
      858119-82-1, 8-(4-Fluorophenylamino)-6-methyl-3,4-
      dihydropyrano[3,4-c]pyridin-1-one 858119-84-3,
      8-(4-Chlorophenylamino)-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one
      858119-85-4 858119-86-5,
      6-Methyl-8-p-tolylamino-3,4-dihydropyrano[3,4-c]pyridin-1-one
      858119-87-6, 6-Methyl-8-phenylamino-3,4-dihydropyrano[3,4-
      c]pyridin-1-one 858119-88-7 858119-89-8
      858119-97-8, 8-Benzylamino-6-methyl-3, 4-dihydropyrano[3, 4-
      c]pyridin-1-one 858119-99-0,
      8-Amino-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-00-0
      858120-01-1 858120-06-6,
      8-Hydroxy-6-methyl-5-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one
      858120-22-6, 8-Methylamino-6-phenyl-3,4-dihydropyrano[3,4-
      c]pyridin-1-one 858120-27-1,
      8-(4-Fluorophenylamino)-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one
      858120-28-2, 8-(4-Methoxybenzylamino)-6-phenyl-3,4-
      dihydropyrano[3,4-c]pyridin-1-one 858120-29-3,
      8-Amino-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-30-6
      858120-31-7 858120-51-1 858120-77-1,
      6-Cyclohexyl-8-(4-methoxybenzylamino)-3,4-dihydropyrano[3,4-c]pyridin-1-
```

ANSWER 1 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

1.6

one 858120-78-2, 8-Amino-6-cyclohexyl-3,4-dihydropyrano[3,4c]pyridin-1-one 858120-83-9, 8-Hydroxy-6-isopropyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-86-2, 6-Isopropyl-8-(4-methoxybenzylamino)-3,4dihydropyrano[3,4-c]pyridin-1-one 858187-08-3 1070913-29-9 1070913-32-4 1070913-33-5 1070913-35-7 1070913-45-9 1070913-48-2 1070913-52-8 1070913-53-9 1070913-54-0 1070913-55-1 1070913-56-2 1070913-57-3 1070913-58-4 1070913-59-5 1070913-60-8 1070913-79-9 1070913-80-2 1070913-81-3 1070913-82-4 1070913-97-1 1070913-98-2 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmaceutical compns. containing lactone type pyridine derivs. as an effective ingredient for prevention and treatment of ischemia) RN 858119-82-1 CAPLUS CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6methyl- (CA INDEX NAME)

RN 858119-84-3 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-chlorophenyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858119-85-4 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[[4-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

RN 858119-86-5 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(4-methylphenyl)amino]- (CA INDEX NAME)

RN 858119-87-6 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-(phenylamino)- (CA INDEX NAME)

RN 858119-88-7 CAPLUS
CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(2-phenylethyl)amino]- (CA INDEX NAME)

RN 858119-89-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(1,3-benzodioxol-5-ylmethyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858119-97-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(phenylmethyl)amino]- (CA INDEX NAME)

RN 858119-99-0 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858120-00-0 CAPLUS

CN Acetamide, N-(3,4-dihydro-6-methyl-1-oxo-1H-pyrano[3,4-c]pyridin-8-yl)(CA INDEX NAME)

RN 858120-01-1 CAPLUS

CN Benzamide, N-(3,4-dihydro-6-methyl-1-oxo-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

RN 858120-06-6 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-methyl-5-phenyl-(CA INDEX NAME)

RN 858120-22-6 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-(methylamino)-6-phenyl- (CA INDEX NAME)

RN 858120-27-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6-phenyl- (CA INDEX NAME)

RN 858120-28-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-phenyl- (CA INDEX NAME)

RN 858120-29-3 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-phenyl- (CA INDEX NAME)

RN 858120-30-6 CAPLUS

CN Acetamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

RN 858120-31-7 CAPLUS

CN Benzamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

RN 858120-51-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-propyl- (CA INDEX

NAME)

RN 858120-77-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-cyclohexyl-3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)

RN 858120-78-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-6-cyclohexyl-3,4-dihydro- (CA INDEX NAME)

RN 858120-83-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-(1-methylethyl)-(CA INDEX NAME)

RN 858120-86-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-(1-methylethyl)- (CA INDEX NAME)

RN 858187-08-3 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-propyl- (CA INDEX NAME)

RN 1070913-29-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 6-ethyl-3,4-dihydro- (CA INDEX NAME)

RN 1070913-32-4 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-ethyl-3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)

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CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-6-ethyl-3,4-dihydro- (CA INDEX NAME)

RN 1070913-35-7 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-(1-methylethyl)- (CA INDEX NAME)

RN 1070913-45-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]-8-(1-methylethyl)- (CA INDEX NAME)

RN 1070913-48-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-cyclohexyl-3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)

RN 1070913-52-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-3,4-dihydro-8-propyl- (CA INDEX NAME)

RN 1070913-53-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]-8-propyl- (CA INDEX NAME)

RN 1070913-54-0 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-3,4-dihydro-8-(1-methylethyl)- (CA INDEX NAME)

RN 1070913-55-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-8-cyclohexyl-3,4-dihydro- (CA INDEX NAME)

RN 1070913-56-2 CAPLUS

CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]-4-fluoro- (CA INDEX NAME)

RN 1070913-57-3 CAPLUS

CN Benzenesulfonamide, 4-chloro-N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]- (CA INDEX NAME)

RN 1070913-58-4 CAPLUS

CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]- (CA INDEX NAME)

RN 1070913-59-5 CAPLUS

CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]-4-methoxy- (CA INDEX NAME)

RN 1070913-60-8 CAPLUS

CN Benzenesulfonamide, N-[3,4-dihydro-8-(1-methylethyl)-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl]-4-methyl- (CA INDEX NAME)

RN 1070913-79-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-ethyl-3,4-dihydro-6-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)

RN 1070913-80-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-amino-8-ethyl-3,4-dihydro- (CA INDEX NAME)

RN 1070913-81-3 CAPLUS

CN Benzenesulfonamide, N-(8-ethyl-3,4-dihydro-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl)-4-fluoro- (CA INDEX NAME)

RN 1070913-82-4 CAPLUS

CN Benzenesulfonamide, N-(8-ethyl-3,4-dihydro-1-oxo-1H-pyrano[3,4-c]pyridin-6-yl)-3-fluoro- (CA INDEX NAME)

RN 1070913-97-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-[(4-fluorophenyl)amino]-3,4-dihydro-8-methyl- (CA INDEX NAME)

RN 1070913-98-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-[(4-chlorophenyl)amino]-3,4-dihydro-8-methyl- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:262396 CAPLUS

DOCUMENT NUMBER: 146:481960

TITLE: A Novel Lumazine Synthase Inhibitor Derived from

Oxidation of 1,3,6,8-Tetrahydroxy-2,7-naphthyridine to

a Tetraazaperylenehexaone Derivative

AUTHOR(S): Zhang, Yanlei; Illarionov, Boris; Bacher, Adelbert;

Fischer, Markus; Georg, Gunda I.; Ye, Qi-Zhuang; Vander Velde, David; Fanwick, Phillip E.; Song,

Yunlong; Cushman, Mark

CORPORATE SOURCE: Department of Medicinal Chemistry and Molecular

Pharmacology, School of Pharmacy and Pharmaceutical

Sciences, and The Purdue Cancer Center, Purdue University, West Lafayette, IN, 47907, USA

SOURCE: Journal of Organic Chemistry (2007), 72(8), 2769-2776

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:481960

AB Air oxidation of 1,3,6,8-tetrahydroxy-2,7-naphthyridine afforded 2,5,8,11-tetraaza-5,11-dihydro-4,10-dihydroxyperylene-1,3,6,7,9,12-hexaone. X-Ray crystallog. of the product revealed that it exists in the meso form in the solid state. The mechanism of product formation most likely involves oxidative phenolic coupling and oxidation. The product proved to be a competitive inhibitor of Schizosaccharomyces pombe lumazine synthase with a Ki of 66 \pm 13 $\mu \rm M$ in Tris buffer and 22 \pm 4 $\mu \rm M$ in phosphate buffer. This is significantly more potent than the naphthyridine reactant (Ki 350 \pm 76 $\mu \rm M$, competitive inhibition), which had previously been identified as a lumazine synthase inhibitor by high-throughput screening. Ab initio calcns. indicate that the meso form is slightly less stable than the enantiomeric form, and that the two forms interconvert rapidly at room temperature

IT 53162-08-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetraazaperylenehexaone by aerial oxidation of tetrahydroxynaphthyridine as lumazine synthase inhibitor and its conformational and mol. docking studies)

RN 53162-08-6 CAPLUS

CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy- (CA INDEX NAME)

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:612303 CAPLUS

DOCUMENT NUMBER: 143:133284

TITLE: Preparation of pyridines as inhibitors of cytokine

production and pharmaceutical compositions containing them useful in the treatment of pain and inflammatory

and immune diseases

Kim, Hyung Ook; Lee, Nam Kyu; Kim, Joo Hyon; Rhee, Hae INVENTOR(S):

In; Cho, Yong-Baik; Ryu, Je Ho; Kim, Nam Ho; Ryu, Keun

Ho; Yi, Jung Bum; Jung, Jae Yoon SK Chemicals, Co. Ltd., S. Korea

SOURCE: PCT Int. Appl., 119 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT NO.					KIND		DATE		APPLICATION NO.						DATE			
WO	WO 2005063768				A1		20050714		WO 2004-KR3545					20041230				
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KΖ,	LC,	LK,	
		LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,	NO,	
		NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ΤJ,	
		TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,	
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	
		MR,	NE,	SN,	TD,	ΤG												
									AU 2004-309303									
CA								CA 2004-2552207										
EP	1706	1706412			A1	20061004			EP 2004-808673						20041230			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,	
		•			•		CY,			CZ,	EE,	HU,	PL,	SK,	IS			
					A 20070328													
BR 2004018301				A	1 20070502				BR 2004-18301					20041230				
									JP 2006-546849									
	2006														_	0060		
			A1	1 20071101				US 2007-585029										
RIORIT	IORITY APPLN. INFO.:												32		A 2			
													45		W 2	0041	230	
THER SO	HER SOURCE(S):						CASREACT 143:133284; MARPAT 143:133284											

E(S)

GΙ

AB The invention is related to novel pyridine derivs. I [wherein R1-R7 = independently H, halo, CN, NO2, acyl, OH, low alkyl, etc.; X = O, S; Y = O, NH and derivs.] and their pharmaceutically acceptable salts having an inhibitory effect on production of cytokines, which are involved in inflammatory responses, and being used as antiinflammatory and analgesic agents. For example, II was prepared by cyclization of 4-(2-hydroxyethyl)-6-methylnicotinonitrile (preparation given) in the presence of concentrated HCl. I showed excellent inhibitory effects on the production of

TNF- α , IL-1 α , IL-6, INF- γ , PGE2. I have shown superiorities in antiinflammatory and analgesic effects over Indomethacin and Celecoxib. Thus, I are useful for treating inflammation and immune diseases.

IT 858119-67-2P, 8-Hydroxy-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1 one 858119-98-9P 858119-99-0P,
 8-Amino-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one

858120-15-7P, 8-Hydroxy-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-28-2P, 8-(4-Methoxybenzylamino)-6-phenyl-3,4-

dihydropyrano[3,4-c]pyridin-1-one 858120-29-3P,

8-Amino-6-phenyl-3, 4-dihydropyrano[3, 4-c]pyridin-1-one

858120-43-1P, 8-Hydroxy-6-propyl-3,4-dihydropyrano[3,4-c]pyridin-1-

one hydrochloride 858120-44-2P,

6-Hydroxy-8-propyl-3,4-dihydropyrano[3,4-c]pyridin-1-one hydrochloride 858120-50-0P, 8-(4-Methoxybenzylamino)-6-(n-propyl)-3,4-

dihydropyrano[3,4-c]pyridin-1-one 858120-51-1P,

8-Amino-6-(n-propyl)-3,4-dihydropyrano[3,4-c]pyridin-1-one

858120-73-7P, 6-Cyclohexyl-8-hydroxy-3,4-dihydropyrano[3,4-

c]pyridin-1-one 858120-77-1P,

6-Cyclohexyl-8-(4-methoxybenzylamino)-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-83-9P, 8-Hydroxy-6-isopropyl-3,4-dihydropyrano[3,4-c]pyridin-1-one

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of cytokine production-inhibiting pyridine derivs.

useful in treating pain and inflammatory and immune diseases)

RN 858119-67-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858119-98-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-methyl- (CA INDEX NAME)

RN 858119-99-0 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858120-15-7 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-phenyl- (CA INDEX NAME)

RN 858120-28-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-phenyl- (CA INDEX NAME)

RN 858120-29-3 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-phenyl- (CA INDEX NAME)

RN 858120-43-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-propyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 858120-44-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-propyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 858120-50-0 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-propyl- (CA INDEX NAME)

RN 858120-51-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-3,4-dihydro-6-propyl- (CA INDEX NAME)

RN 858120-73-7 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 6-cyclohexyl-3,4-dihydro- (CA INDEX NAME)

RN 858120-77-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 6-cyclohexyl-3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]- (CA INDEX NAME)

RN 858120-83-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-(1-methylethyl)-(CA INDEX NAME)

ΙT 858119-64-9P, 6,8-Dihydroxy-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-82-1P, 8-(4-Fluorophenylamino)-6-methyl-3,4dihydropyrano[3,4-c]pyridin-1-one 858119-84-3P, 8-(4-Chlorophenylamino)-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-85-4P, 8-[(4-Trifluoromethylphenyl)amino]-6-methyl-3,4dihydropyrano[3,4-c]pyridin-1-one 858119-86-5P, 6-Methyl-8-(p-tolylamino)-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-87-6P, 6-Methyl-8-phenylamino-3,4-dihydropyrano[3,4c]pyridin-1-one 858119-88-7P, 6-Methyl-8-[(2-phenylethyl)amino]-3,4-dihydropyrano[3,4-c]pyridin-1-one 858119-89-8P, 8-[(Benzodioxol-5-ylmethyl)amino]-6-methyl-3,4dihydropyrano[3,4-c]pyridin-1-one 858119-97-8P, 8-Benzylamino-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-00-0P, 8-Acetamido-6-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-01-1P, N-(1-Oxo-6-methyl-3,4-dihydropyrano[3,4c]pyridin-8-yl)benzamide 858120-06-6P, 8-Hydroxy-6-methyl-5-phenyl-3, 4-dihydropyrano[3, 4-c]pyridin-1-one 858120-22-6P, 8-Methylamino-6-phenyl-3,4-dihydropyrano[3,4c]pyridin-1-one 858120-27-1P, 8-(4-Fluorophenylamino)-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-30-6P, 8-Acetamido-6-phenyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-31-7P, N-(1-0xo-6-phenyl-3,4-dihydropyrano[3,4c]pyridin-8-yl)benzamide 858120-34-0P, 6-Hydroxy-8-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one hydrochloride 858120-52-2P, N-[1-0xo-6-(n-propyl)-3,4-dihydro-1H-pyrano[3,4c]pyridin-8-yl]acetamide 858120-78-2P, 8-Amino-6-cyclohexyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-86-2P, 6-Isopropyl-8-(4-methoxybenzylamino)-3,4dihydropyrano[3,4-c]pyridin-1-one 858120-87-3P, 6-Hydroxy-8-methyl-3,4-dihydropyrano[3,4-c]pyridin-1-one 858120-88-4P, 8-Hydroxy-6-(n-propyl)-3,4-dihydropyrano[3,4-c]pyridin-1-one RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of cytokine production-inhibiting pyridine derivs.

useful in treating pain and inflammatory and immune diseases)

RN 858119-64-9 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-hydroxy- (CA INDEX NAME)

RN 858119-82-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858119-84-3 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-chlorophenyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858119-85-4 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[[4-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

RN 858119-86-5 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(4-methylphenyl)amino]- (CA INDEX NAME)

RN 858119-87-6 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-(phenylamino)- (CA INDEX NAME)

RN 858119-88-7 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(2-phenylethyl)amino]- (CA INDEX NAME)

RN 858119-89-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(1,3-benzodioxol-5-ylmethyl)amino]-3,4-dihydro-6-methyl- (CA INDEX NAME)

RN 858119-97-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-6-methyl-8-[(phenylmethyl)amino]- (CA INDEX NAME)

RN 858120-00-0 CAPLUS

CN Acetamide, N-(3,4-dihydro-6-methyl-1-oxo-1H-pyrano[3,4-c]pyridin-8-yl)-(CA INDEX NAME)

RN 858120-01-1 CAPLUS

CN Benzamide, N-(3,4-dihydro-6-methyl-1-oxo-1H-pyrano[3,4-c]pyridin-8-yl)-(CA INDEX NAME)

RN 858120-06-6 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-methyl-5-phenyl-(CA INDEX NAME)

RN 858120-22-6 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-(methylamino)-6-phenyl- (CA INDEX NAME)

RN 858120-27-1 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-[(4-fluorophenyl)amino]-3,4-dihydro-6-phenyl- (CA INDEX NAME)

RN 858120-30-6 CAPLUS

CN Acetamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

RN 858120-31-7 CAPLUS

CN Benzamide, N-(3,4-dihydro-1-oxo-6-phenyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

RN 858120-34-0 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 858120-52-2 CAPLUS

CN Acetamide, N-(3,4-dihydro-1-oxo-6-propyl-1H-pyrano[3,4-c]pyridin-8-yl)- (CA INDEX NAME)

RN 858120-78-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 8-amino-6-cyclohexyl-3,4-dihydro- (CA INDEX NAME)

RN 858120-86-2 CAPLUS

CN 1H-Pyrano[3,4-c]pyridin-1-one, 3,4-dihydro-8-[[(4-methoxyphenyl)methyl]amino]-6-(1-methylethyl)- (CA INDEX NAME)

RN 858120-87-3 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,6(7H)-dione, 3,4-dihydro-8-methyl- (CA INDEX NAME)

RN 858120-88-4 CAPLUS

CN 1H-Pyrano[3,4-c]pyridine-1,8(7H)-dione, 3,4-dihydro-6-propyl- (CA INDEX NAME)

REFERENCE COUNT:

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:41677 CAPLUS

DOCUMENT NUMBER: 138:337967

TITLE: Studies with alkylheterocycles: novel synthesis of

functionally substituted isoquinoline and

pyridopyridine derivatives

AUTHOR(S): Elmaati, Tarek M. Abu; El-Taweel, Fathy M. A.

CORPORATE SOURCE: Faculty of Specific Education, New Damietta, Mansoura

University, Egypt

SOURCE: Journal of the Chinese Chemical Society (Taipei,

Taiwan) (2002), 49(6), 1045-1050 CODEN: JCCTAC; ISSN: 0009-4536

PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:337967

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Reaction of cyanopyridinone I with cinnamonitriles gave isoquinolines such as II $[R = (un)substituted\ phenyl]$. Treating I with elemental sulfur yielded thienopyridine III. III reacted with acrylonitrile to give isoquinoline II (R = H). II (R = H) was also prepared from I and methylenemalononitrile. Condensation of I with benzaldehyde, followed by treatment with NH4OH or AcOH/HCl gave pyridopyridine IV or V.

IT 517907-24-3P 517907-25-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (conversion of cyanopyridinone derivative to isoquinolinones, thienopyridinone, and pyridopyridines by reactions with unsatd. nitriles, sulfur, or benzaldehyde)

RN 517907-24-3 CAPLUS

CN 2,7-Naphthyridine-4-carboxamide, 8-amino-N-(4-chlorophenyl)-1,2-dihydro-1-oxo-6-phenyl- (CA INDEX NAME)

RN 517907-25-4 CAPLUS

CN 2,7-Naphthyridine-4-carboxamide, N-(4-chlorophenyl)-1,2,7,8-tetrahydro-1,8-dioxo-6-phenyl- (CA INDEX NAME)

REFERENCE COUNT:

7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:501464 CAPLUS

DOCUMENT NUMBER: 137:352926

TITLE: 1-(N, N-dimethylamino)-2-(N-phenylcarbamoyl)-1-buten-3-

one as a building block for the synthesis of

heterocyclic compounds

AUTHOR(S): Elmaati, T. A.; Said, S.; Elenein, N. A.; Sofan, M.;

Khodeir, N.

CORPORATE SOURCE: Faculty of Specific Education, Mansoura University,

New Damietta, Egypt

SOURCE: Polish Journal of Chemistry (2002), 76(7), 945-952

CODEN: PJCHDQ; ISSN: 0137-5083

PUBLISHER: Polish Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:352926

AB Acetoacetanilide reacted with DMF-DMA to give the enaminone MeCOC(:CHNMe2)CONHPh (I). I, when treated with hydrazines, gives pyrazoles, resp., and with pyrazole derivs. the pyrazolopyrimidines. On the other hand, in reaction of I with benzimidazole and benzimidazole-2-acetonitrile, pyrimidobenzimidazole and the pyridobenzimidazole were formed. I reacts with hippuric acid in boiling acetic anhydride to afford a pyridine derivative In the reaction of I with malononitrile, cyanoacetamide or malononitrile dimer compds. were formed.

IT 474369-52-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (use of (N,N-dimethylamino)(N-phenylcarbamoyl)butenone as a building block for the synthesis of heterocyclic compds.)

RN 474369-52-3 CAPLUS

CN 2,7-Naphthyridine-4-carboxamide, 1,2,7,8-tetrahydro-1,8-dioxo-N-phenyl-(CA INDEX NAME)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:61571 CAPLUS

DOCUMENT NUMBER: 116:61571

ORIGINAL REFERENCE NO.: 116:10627a, 10630a

TITLE: Heterocyclic compounds and their use as dyes and

pigments

INVENTOR(S): Hoechstetter, Hans
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3937633	A1	19910516	DE 1989-3937633	19891111
US 5097027	A	19920317	US 1990-593460	19901005
EP 427993	A2	19910522	EP 1990-120651	19901027
EP 427993	A3	19920122		
R: CH, DE, FR,	GB, LI			
JP 03181567	A	19910807	JP 1990-299089	19901106
PRIORITY APPLN. INFO.:			DE 1989-3937633 A	19891111
OTHER SOURCE(S):	MARPAT	116:61571		
GT				

AB The dyes and pigments are I and II (R1-R4 = H, alkyl, cycloalkyl, aryl, aralkyl, heteroaryl; R5 = halogen, NR1R2, SR1, OR1, aryl, heteroaryl, OX; X = cation; when R-R4 = H, R5 \neq OH, ONa). Thus, 29 g 2,7-naphthyridine-1,3,6,8-tetraol di-Na salt in 90 mL MeC6H4SO3Me was heated 12.5 h at 190°, cooled to 100°, and precipitated in MeOH to give 23 g I-II mixture (R1-R4 = Me; R5 = OH) (III). III was a reddish violet pigment with good migration resistance.

IT 137219-69-3

RL: USES (Uses)

(alkylation-dimerization of, in manufacture of pigments and dyes)

RN 137219-69-3 CAPLUS

CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy-, sodium salt (1:2) (CA INDEX NAME)

●2 Na

L6 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1974:437490 CAPLUS

DOCUMENT NUMBER: 81:37490
ORIGINAL REFERENCE NO.: 81:6003a,6006a

TITLE: Condensation of dicarbonyl compounds with

malononitrile. VIII. Condensation of malononitrile

with some esters of $\beta\text{-keto}$ acids

AUTHOR(S): Gudriniece, E.; Rigerte, B. CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR

SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija

(1974), (2), 239-40

CODEN: LZAKAM; ISSN: 0002-3248

DOCUMENT TYPE: Journal LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB Nicotinonitriles I (R = Me, Ph) were obtained in 56% and 20% yields, resp., by condensing malononitrile with RCOCH2CO2Et to give intermediate RC(CH2CO2Et):C(CN)2 which were cyclized by 70% HClO4. Analogously obtained was 77% naphthyridine II from malononitrile and (EtO2CCH2)2CO.

IT 53162-08-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 53162-08-6 CAPLUS

CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy- (CA INDEX NAME)

L6 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1973:466219 CAPLUS

DOCUMENT NUMBER: 79:66219

ORIGINAL REFERENCE NO.: 79:10699a,10702a
TITLE: Simple synthesis of

1-hydroxy-3-naphthyridinecarboxylic acid

AUTHOR(S): Trommer, Wolfgang; Blume, Heinrich

CORPORATE SOURCE: Abt. Chem., Ruhr Univ., Bochum, Fed. Rep. Ger.

SOURCE: Tetrahedron Letters (1973), (17), 1447-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: German

GI For diagram(s), see printed CA Issue.

Condensation of 3-cyano-4-methylpyridine (prepared by heating the 3-bromo analog with CuCN) with (CO2Et)2 using Me3COK as base gave the cyano ester (I) which gave the title compound (II) on hydrolysis. The 7-Me analog of II was prepared in 80% yield by 1,4-addition of MeCOCO2H to N-methylnicotinamide chloride followed by oxidation with p-ONC6H4NMe2 or (Cl3C)2CO.

IT 42285-32-5P 42285-33-6P

RN 42285-32-5 CAPLUS

CN 2,7-Naphthyridinium, 6-carboxy-7,8-dihydro-2-methyl-8-oxo-, inner salt (CA INDEX NAME)

RN 42285-33-6 CAPLUS

CN 2,7-Naphthyridinium, 6-carboxy-7,8-dihydro-2-methyl-8-oxo-, chloride (1:1) (CA INDEX NAME)

L6 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:435253 CAPLUS

DOCUMENT NUMBER: 73:35253
ORIGINAL REFERENCE NO.: 73:5841a,5844a

TITLE: Reactions of some 4-methylene-4H-pyran derivatives

with primary and secondary amines

AUTHOR(S): Van Allan, James A.; Reynolds, George Arthur;

Petropoulos, C. C.; Maier, D. P.

CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA SOURCE: Journal of Heterocyclic Chemistry (1970), 7(3),

495-507

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 73:35253

AB 4-Dicyanomethylene-4H-pyrans react with secondary amines to give 2-aminopyridine and 2-pyridone derivs., which, in turn, were used to prepare copyrine derivatives. These pyrans and pyrimary amines gave copyrine and iminopyridone derivatives in addition to

 ${\tt dicyanomethylene-1,4-dihydropyridines.} \quad {\tt Reaction of} \\$

cyanocarbamoylmethylene-4H-pyrans with secondary amines gave 2-pyrones, and with primary amines, gave copyrines and 1,4-dihydropyridine derivs.

IT 27337-84-4P 27337-98-0P 27338-00-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 27337-84-4 CAPLUS

CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-diphenyl- (CA INDEX NAME)

RN 27337-98-0 CAPLUS

CN 2,7-Naphthyridin-1(2H)-one, 8-(butylamino)-3,6-diphenyl- (CA INDEX NAME)

RN 27338-00-7 CAPLUS

CN 2,7-Naphthyridin-1(2H)-one, 3,6-diphenyl-8-[(phenylmethyl)amino]- (CA INDEX NAME)

L6 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:11376 CAPLUS

DOCUMENT NUMBER: 64:11376
ORIGINAL REFERENCE NO.: 64:2046c-d

TITLE: Condensations of carbonyl compounds at the methyl or

 $\alpha\text{-methylene}$ group of 6- or

4-alkyl-3-cyano-2(1)-pyridones through dianions

AUTHOR(S): Boatman, Sandra; Harris, Thomas M.; Hauser, Charles R.

CORPORATE SOURCE: Duke Univ., Durham, NC

SOURCE: Journal of the American Chemical Society (1965),

87(22), 5198-202

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 64:11376

AB Several types of condensations of carbonyl compds. at the methyl or methylene group of 6- or 4-alkyl-3-cyano-2(1)-pyridones were effected through dianions, which were prepared by means of 2 mole-equivs. of potassium amide in liquid ammonia. The types of condensations realized were aroylation with methyl benzoate, acylation with ethyl oxalate, carbonyl addition with benzophenone or benzaldehyde, and conjugate addition with chalcone. One of the benzoyl derivs. was converted by polyphosphoric acid to the corresponding amide and another to a dihydroxy-2,7-naphthyridine. The carbonyl addition products were dehydrated or converted to another derivative Consideration is given to possible extensions of the method.

IT 27337-84-4P, 2,7-Naphthyridine-1,8-diol, 3,6-diphenyl-

RL: PREP (Preparation)

(preparation of)

RN 27337-84-4 CAPLUS

CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-diphenyl- (CA INDEX NAME)

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ANSWER 11 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
1.6
                         1961:13414 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         55:13414
ORIGINAL REFERENCE NO.: 55:2640b-f
TITLE:
                         Some derivatives of 2,7-naphthyridine
                         Ferrier, B. M.; Campbell, Neil
AUTHOR(S):
CORPORATE SOURCE:
                         Univ. Edinburgh, UK
                         Journal of the Chemical Society (1960) 3513-15
SOURCE:
                         CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         Unavailable
     The synthesis of some 2,7-naphthyridine derivs. was described. CH2(CN)2
     (1 g.) kept 19 days with 3 g. CO(CH2CO2Et)2 in 25 ml. alc. containing 4 drops
     NHEt2 gave 2.6 g. di-Et \beta-(dicyanomethylene)glutarate, yellow
     needles, m. 166^{\circ} (C6H6). CH2(CN)2 (1.1 g.) was condensed with
     CO(CH2CO2Et)2 as above; after 24 hrs. no ketone could be detected and
     after a further 24 hrs. the solvent removed, the residue warmed 30 sec.
     with 20 ml. 70% H2SO4, then refluxed 30 sec., cooled, and poured into 60
     ml. H2O gave 2.7 g. 1,3,6,8-tetrahydroxy-2,7-naphthyridine (I), m. above
     350°; dibenzoate m. 234-9°; dinitroso compound m. above
     350^{\circ}. I (1 g.) heated 24 hrs. at 180^{\circ} in a sealed tube with
     10 ml. POCl3, the mixture poured on 150 g. ice, made alkaline, and extracted
with
     Et20 gave 0.5 g. 1,3,6,8-tetrachloro-2,7-naphthyridine (II), yellow
     needles, m. 157-61^{\circ} (aqueous alc.). The residue after extraction with
     ligroine gave 0.1 g. 1,3,8-trichloro-8-hydroxy-2,7-naphthyridine, m.
     295\,^{\circ} (C6H6). II (0.46 g.), 1 g. fused KOAc, and 0.2 g. PdCl2 in 40
     ml. MeOH shaken with H, the oily residue dissolved in H2O, made alkaline, and
     extracted with EtOAc gave 0.04 g. 1,2,3,4-tetrahydro-2,7-naphthyridine
     picrate, orange-yellow prisms, m. 248-50° (H2O). II (0.36 g.), 0.2
     g. PdCl2, and 1 g. anhydrous K2CO3 in 25 ml. MeOH shaken 1 hr. with H gave
     0.014 g. 1,8-dimethoxy-2,7-naphthyridine, m. 108-10°; picrate,
     yellow blades, m. 148-50° (C6H6). From the MeOH filtrate
     tetrahydro-2,7-naphthyridine was isolated as the picrate. II (0.1 g.) in
     5 \text{ ml.} MeOH with 0.1 \text{ g.} anhydrous K2CO3 afforded after 1 \text{ hr.}
     3,6-dichloro-1,8-dimethoxy-2,7-naphthyridine (III), needles, m.
     155-7^{\circ} (MeOH). III (0.08 g.) was obtained when 0.1 g. II was
     refluxed 1 hr. in 5 ml. MeOH with 5 ml. 10% aqueous K2CO3. NCCH2CO2Et (2.5
     q.), 4 q. CO(CH2CO2Et)2, and 6 drops EtNH2 kept 7 days in 10 ml. alc., the
    mixture evaporated, the residue (3.2 g.) kept overnight in 20 ml. concentrated
H2SO4,
     and poured into H2O gave 1.4 g. Et
     3-ethoxycarbonyl-2,6-dihydroxy-4-pyridylacetate, orange-yellow needles, m.
     176.5° (alc.). CH2(CN)2 (0.35 g.), 0.43 g. Et2CO, and 2 drops
     NHEt2 kept 4 days in 2 ml. alc. gave 0.06 g.
     2-cyano-3-ethyl-2-pentenonitrile, m. 160-1° (aqueous alc.). Dibenzyl
     ketone (1.5 g.) after 12 hrs. gave 1.15 g.
     3-benzyl-2-cyano-4-phenyl-2-butenonitrile, plates, m. 49.5° (aqueous
     alc.). Me2CO and fluorenone gave corresponding products, m. 172-3^{\circ}
     and 234^{\circ}, resp.
ΙT
     53162-08-6P, 1,3,6,8-Copyrinetetrol 114698-11-2P,
     1,3,6,8-Copyrinetetrol, 4,5-dinitroso-(?) 116083-61-5P,
     1,3,6,8-Copyrinetetrol, dibenzoate
     RL: PREP (Preparation)
        (preparation of)
     53162-08-6 CAPLUS
RN
CN
     2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy- (CA INDEX NAME)
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RN 114698-11-2 CAPLUS

CN 2,7-Naphthyridine-1,8(2H,7H)-dione, 3,6-dihydroxy-4,5-dinitroso- (CA INDEX NAME)

RN 116083-61-5 CAPLUS

CN 1,3,6,8-Copyrinetetrol, dibenzoate (6CI) (CA INDEX NAME)

CM 1

CRN 53162-08-6 CMF C8 H6 N2 O4

CM 2

CRN 65-85-0 CMF C7 H6 O2

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ANSWER 12 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
1.6
ACCESSION NUMBER:
                         1958:88095 CAPLUS
DOCUMENT NUMBER:
                         52:88095
ORIGINAL REFERENCE NO.: 52:15532a-i
TITLE:
                         2,7-Naphthyridine derivatives
                         Birkofer, Leonhard; Kaiser, Christelmargot
AUTHOR(S):
CORPORATE SOURCE:
                         Univ. Cologne, Germany
                         Chemische Berichte (1957), 90, 2933-40
SOURCE:
                         CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE:
                         Journal
                         Unavailable
LANGUAGE:
    N-Methyl-3-aminoformylpyridinium chloride (I) condensed with Me2CO in alkaline
     solution by the method of Huff (C.A. 41, 2738b), the mixture worked up, and the
     crude product treated with HCl gave
     3,7-dimethyl-1-oxo-1,7-dihydroxy-2,7-naphthyridine.HCl (II), yellowish
     prisms, m. 320-2^{\circ} (decomposition). II (2 g.) heated at
     290-300^{\circ}/0.1-0.2 and the sublimate recrystd. (H2O) gave 75-90\%
     3-methyl-1-oxo-1,2-dihydro-2,7-naphthyridine (III), rods, m. 264°
     (H2O). I (7.5 \text{ g.}) in 195 cc. H2O and 195 cc. Me2CO treated with stirring
     with 24 cc. 7N KOH, kept 12 hrs. at room temperature, treated with 45 cc.
concentrated
     HCl, heated 20 min. in an H2O bath, and evaporated in vacuo, the yellow
     residue heated 1 hr. at 50° with a little EtOH and kept 24 hrs. at
     -20°, and the deposit filtered, washed with EtOH, dried, and
     sublimed at 290°/0.1-0.2 yielded about 20% III. III in MeOH
     treated with diphenyldisulfimide (IV) gave III.IV adduct, needles, m.
     214°. Similarly was prepared the p,p'-dichlorodiphenyldisulfimide
     derivative of III, m. 175°. III, in MeOH treated with aqueous picric acid
     gave the picrate of III, yellow needles, m. 234^{\circ} (decomposition). III
     refluxed with MeI gave III.MeI, scales, m 309° (decomposition) (aqueous
    MeOH). III.MeI with AqCl gave II. The recrystn. mother liquors from III
     basified slightly with aqueous Na2CO3 and evaporated in vacuo, the residue
     sublimed at 300^{\circ}/0.1-0.2, the resinous brown precipitate dissolved in H2O,
     the solution adjusted to pH 4, passed through Amberlite IR-4B, and extracted
with
    CHCl3, the extract evaporated, and the residue distilled gave 2-Me derivative
of III, m.
     138° (MeOH-Et20); HCl salt, m. 283-6° (decomposition) (MeOH).
     III (3 q.) in absolute MeOH treated with excess CH2N2-Et2O, refrigerated 5
     weeks, filtered, and evaporated, the residue boiled with H2O, and the aqueous
     worked up gave the N-Me derivative of III, needles, m. 137-8° (picrate,
     leaflets, m. 217°); the H2O-insol. material (volatile with steam)
     recrystd. (petr. ether) gave 1-methoxy-3-methyl-2,7-naphthyridine, (V)
     needles, m. 92° (petr. ether). III (2 g.) and 20 cc. POCl3 heated
     1 hr. at 140-5^{\circ} in a sealed tube, cooled, filtered, and evaporated in
     vacuo, the residue basified with saturated aqueous Na2CO3 and extracted with
CHC13,
     and the extract worked up gave an oil-crystal mixture which sublimed at
     95-100°/12 yielded 70% 1-chloro-3-methyl-2,7-naphthyridine (VI),
     leaflets, m. 106° (petr. ether); picrate, m. 157° (MeOH).
     VI (750 mg.) in a little absolute MeOH added to NaOMe solution, refluxed 1 hr.,
     and evaporated in vacuo, and the residue decomposed with iced H2O, the
precipitate
     dissolved in EtOAc, dried, and evaporated, and the residue recrystd. (petr.
     ether) yielded V, needles, m. 92°. VI (4.5 g.) heated 2 hrs. at
     150^{\circ} with 15 cc. Et2N(CH2)2NH2, the excess amine distilled, the
     residue dissolved in dilute aqueous KOH and extracted with Et20, and the
extract worked
     up gave 1-(Et2N CH2CH2NH) analog of V, yellow viscous oil, b0.012
     138-40°; HCl salt, deliquescent crystals, showed in MeOH green
     fluorescence; dipicrate, yellow leaflets, m. 183° (decomposition)
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(MeOH); monopicrate, orange prisms, m. $183-4^{\circ}$ (H2O). VI in MeOH hydrogenated over 10 weight-% 1% Pd-CaCO3, filtered, and evaporated, the residue

dissolved in H2O, the solution basified with Na2CO3, treated with NaCl, and extracted with CHCl3, and the extract worked up gave 40-50% 3-methyl-2,7-naphthyridine, deliquescent crystals, m. 39°, b0.12 76°; picrate, yellow needles, m. 219-21° (H2O). III (3 g.) in 50 cc. concentrated HNO3 (d. 1.4) heated 8 hrs. on the H2O bath with the occasional addition of a few cc. HNO3 and concentrated at 20 mm., the residue treated with H2O, the precipitate dried and refluxed 20 min. with Ac2O, and the mixture distilled yielded the anhydride of cinchomeronic acid (VII), b12 139-42°, m. 73°, which heated with H2O gave VII, m. 268° (decomposition). The anhydride of VII with EtOH gave the γ-Et ester of VII, prisms, m. 128-31° (EtOAc-ligroine). 112689-01-7P, 7,8-Dihydro-2,6-dimethyl-8-oxocopyrinium iodide RL: PREP (Preparation) (preparation of)

2,7-Naphthyridinium, 3,7-dimethyl-1-oxo-, iodide (1:1) (CA INDEX NAME)

112689-01-7 CAPLUS

ΙT

RN

CN

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ANSWER 13 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
1.6
ACCESSION NUMBER:
                         1957:51897 CAPLUS
DOCUMENT NUMBER:
                          51:51897
ORIGINAL REFERENCE NO.: 51:9641b-i,9642a-f
                         Structure of gentianine
TITLE:
                         Govindachari, T. R.; Nagarajan, K.; Rajappa, S.
AUTHOR(S):
CORPORATE SOURCE:
                         Presidency Coll., Madras
                         Journal of the Chemical Society (1957) 551-6
SOURCE:
                         CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         Unavailable
     cf. C.A. 51, 5070c. Powdered Enicostemma littorale (2 kg., from whole plant)
     made into a paste with 2 l. NH4OH (d. 0.9) and H2O, dried at 30^{\circ} in
     the shade, extracted several hrs. with CHC13, the extract shaken with N H2SO4,
     the acid extract neutralized with BaCO3 and filtered, the filtrate acidified
     with AcOH, concentrated, made alkaline with NH4OH, extracted thoroughly with
     the crude product on evaporation (6-12 g.) crystallized from moist Et2O gave
4-8 g.
     gentianine (I), m. 82-3°, [\alpha]D30 \pm 0^{\circ} (CHCl3),
     \lambda 220, 245, 280 m\mu (log \epsilon 4.38, 3.9, 3.2), \nu 1719
     (\alpha\beta-unsatd. \delta-lactone), 1634 (conjugated double bond)
     cm.-1, with no bands in the 1300-1400 cm.-1 (C-methyl) region, no C-Me
     group by Kuhn-Roth method; HCl salt, m. 169-70° (decomposition); HBr
     salt, m. 178° (decomposition); HNO3 salt, m. 113° (decomposition);
     oxalate, m. 123-4^{\circ}; (+)-tartrate, m. 138^{\circ}; picrate, m.
     123-4^{\circ}; methiodide, m. 193^{\circ}. In general the m.p. of the
     salts agree with those given by Proskurnina, et al. (C.A. 40, 72132; 44,
     159d). Treatment with alc. NaOH gave a Na salt from which I was recovered
     on acidification. I (0.8 g.) in 25 ml. MeOH shaken with H at 55 lb./sq.
     in. in the presence of PtO2 and the product crystallized from Et2O-petr. ether
     gave 0.6 g. dihydrogentianine, m. 74-6°, \lambda 270 m\mu (log
     \varepsilon 3.4); picrate, m. 140-2°. I (0.5 g.) ozonized 6 hrs. in
     50 ml. dry CHC13 at 0^{\circ}, the mixture evaporated in vacuo at 30^{\circ} and
     the residue refluxed 1 hr. with 100 ml. H2O, the solution diluted with 100 ml.
     H2O and 1 ml. AcOH, steam distilled into 200 ml. H2O containing 1.5 g. dimedon,
     the distillate boiled, filtered hot, and the solution cooled gave
     HCHO-Me2C6H6O2, m. 187°. Oxidation of 1.45 g. I in 50 ml. Me2CO
     with 4.4 g. KMnO4 in 300 ml. Me2CO produced 0.94 g.
     4-(2-hydroxyethyl)pyridine-3,5-dicarboxylic acid lactone (II), m.
     260-2°, \lambda 265 m\mu (log \epsilon 3.1), showing the
     presence of a vinyl group. Vigorous oxidation of 0.5 g. I in 20 ml. 2N
     NaOH at 100° with 2 g. KMnO4 in 20 ml. H2O, working up the product,
     and purifying by passage through Zeo-Karb 315 gave
     pyridine-3,4,5-tricarboxylic acid, m. 262-4°, also obtained by
     oxidation of 5-ethyl-4-methylnicotinic acid (III). II (0.94 g.) in 3 ml.
     H2O containing 0.55 g. KOH evaporated and the salt distilled with 3 g.
soda-lime gave
     crude base (picrate, m. 155-6°), oxidized (100 g.) in 20 ml. H2O
     containing 1 ml. 2N NaOH at 100° with 0.3 g. KMnO4, the solution filtered,
     the filtrate and hot H2O washings acidified and evaporated, the residue
extracted
     with boiling alc. yielding isonicotinic acid (picrate, m. 215°),
     thus establishing the alc. side chain in position 4. Two alternative
     structures for I given by these degradations were evaluated by synthesis
     since attempts to decarboxylate the acid from the I dihydro derivative were
     unsuccessful. The simpler 4-(1-hydroxyethyl)-nicotinic acid lactone (IV)
     was first synthesized to determine the exptl. conditions. EtCOCH2CO2Et (9 g.),
     5 g. NCCH2CONH2, 10 ml. piperidine, and 15 ml. MeOH refluxed 3 hrs., the
     MeOH evaporated, and the residue in 50 ml. H2O acidified with dilute HCl
yielded
     3 g. 3-cyano-2,6-dihydroxy-4-ethylpyridine. The nitrile (9 g.) heated 4
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hrs. at 180° with 18 ml. POC13 in a sealed tube, the cooled mixture
     poured onto cracked ice, the solution extracted at room temperature with Et20,
the
     dried extract evaporated and the crude chloro compound (8 g.) hydrogenated 30
min.
     at 2 atmospheric in 100 ml. MeOH containing 10 g. KOAc and 0.7 g. PdCl3, the
filtered
     solution evaporated, the residue in 50 ml. H2O saturated with NaHCO3 and
extracted with
     Et20, the dried extract evaporated, and the residue distilled in vacuo gave
     4-ethylnicotinonitrile, b3.5 92-3° (picrate, m. 153-5°),
     hydrolyzed to 4-ethylnicotinic acid. The acid (0.85 g.) in 6 ml. AcOH
     containing 2 ml. 30% H2O heated 3 hrs. at 70^{\circ}, treated with 2 ml. 30%
     H2O, and kept 8 hrs. at 70°, the solution evaporated in vacuo and the
     residue recrystd. twice from H2O gave 0.85 g. N-oxide, m. 187-8°,
     converted by refluxing 4 hrs. in dioxane containing Ac20 to
     4-(1-hydroxyethyl) pyridine acetate (picrate, m. 148-51^{\circ}) and IV, m.
     87-8°, \lambda 255 m\mu (log \epsilon 3.18) (picrate, m.
     153°), also obtained by warming 0.5 g. acid into solution with 2 ml.
     Ac20 and keeping the mixture overnight at 30°. Similarly,
     4,5-diethylnicotinic acid (V) was synthesized from EtCOCHEtCO2Et (VI). VI
     (22 g.) shaken 6 days with 40 ml. NH4OH (d. 0.9), the aqueous layer separated
and
     treated with 16 ml. NCCH2CO2Et, filtered after standing 4 days at
     30°, the residual salt taken up in H2O and the solution acidified,
     filtered, and the residue recrystd. from H2O gave 7 g.
     3-cyano-4,5-diethyl-2,6-dihydroxypyridine (VII), m. 186-7°
     (decomposition). VII (10 g.) heated with 20 ml. POCl3 gave 8 g. chloro
compound,
     hydrogenated in 100 ml. MeOH containing 8 g. KOAc and 0.7 g. PdCl4 to give 3.2
     g. 4,5-diethylnicotinonitrile, b. 110° (picrate, m.
     144.0-5.5^{\circ}), which heated 6 hrs. at 140^{\circ} with 32 ml. 75%
     H2SO4, the iced mixture treated with Ca(OH)2 to pH 5-6, filtered, the
     filtrate and washings evaporated in vacuo, the residue extracted with alc., the
     extract evaporated and the residual amino acid sulfate taken up in H2O and
     through De-Acidite E, the eluate evaporated, and the residue recrystd. from
     alc.-Et20 gave 2.5 g. V, m. 115-16°; N-oxide, m. 190-2°.
     The oxide (0.5 g.) shaken with 2 ml. warm Ac2O, the dark red solution worked
     up to give 180 mg. red oily 5-ethyl-4-(1-hydroxyethyl)nicotinic acid
     lactone; picrate, m. 148-9°, \nu 1763 cm.-1
     (\alpha, \beta-unsatd. \gamma-lactone), differing from that of
     dihydrogentianine picrate, m. 140-2°, \nu 1720 cm.-1, and so
     eliminating the structure proposed by P., et al. (loc. cit.), for I.
     POC13 (10 ml.) heated 4.5 hrs. at 160° with 5 g.
     3-cyano-2,6-dihydroxy-5-ethyl-4-methylpyridine [from AcCHEtCO2Et (cf.
     Ruzicka and Fomasir, C.A. 13, 3179)] gave 4.5 g.
     3-cyano-2,6-dichloro-5-ethyl-4-methylpyridine, hydrogenated in 50 ml. MeOH
     containing 0.4 g. PdCl4 and 5.5 g. KOAc to yield 2.5 g.
     5-ethyl-4-methylnicotinonitrile, b7 120° (picrate, m.
     157-8°), hydrolyzed with 75% H2SO4 and worked up to give
     5-ethyl-4-methylnicotinic acid (VIII), m. 163-5^{\circ}. VIII (1 g.) and 3 ml. 40% HCHO heated 24 hrs. at 100^{\circ} in a sealed tube, excess HCHO
     removed by steam distillation, the solution concentrated to 5 ml. and
extracted with
     CHCl3Et20, the dried extract evaporated and the Et20-washed residue
crystallized from
     MeOH-Et20 gave 2-(3-carboxy-5-ethyl-4-pyridyl)propane-1,3-diol lactone
     (IX), m. 168-9°, identical with that obtained by similar treatment
     of dihydrogentianine, m. 74-6^{\circ}, synthesized by heating 0.5 g. VIII
     Na salt 15 hrs. at 100° with 0.3 ml. 40% HCHO and fractionating the
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crude product from petr. ether, together with IX. The structure of I is conclusively established and the identity of I from E. littorale and gentianine confirmed. The alkaloid erythricine (C.A. 41, 7676c) may also prove to be identical with I.

IT 117885-38-8

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 117885-38-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridinium, 5-ethenyl-3,4-dihydro-7-methyl-1-oxo-, iodide (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH} & \text{CH}_2 \\ \hline \\ \text{O} & \text{N}^+ \\ \\ \text{O} & \\ \end{array}$$

• I-

L6 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1957:51896 CAPLUS

DOCUMENT NUMBER: 51:51896

ORIGINAL REFERENCE NO.: 51:9640b-i,9641a-b

TITLE: Taraxanthin and tarachrome. Stereoisomeric

trollixanthins

AUTHOR(S): Eugster, C. H.; Karrer, P.

CORPORATE SOURCE: Univ. Zurich, Switz.

SOURCE: Helvetica Chimica Acta (1957), 40, 69-79

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB Pure crystalline taraxanthin (I) (cf. Kuhn and Lederer, C.A. 21, 750) has been isolated from Bundner Rheintal summer crop yellow balsam (Impatiens noli-tangere) by a modification of the procedure of K. and L. Shade-dried blossoms (5500) (45.5 g.) warmed gently with C6H6, kept overnight and decanted, the extraction repeated and the material dried in vacuo at 40°, milled and again extracted with C6H6, the combined exts. evaporated in vacuo (N atmospheric), the viscous oily residue taken up in 70 cc. C6H6, treated

with 6.5 g. KOH in 50 cc. alc. and some petr. ether, the mixture kept 8 hrs. at room temperature and warmed 45 min. at 70° , the cooled mixture diluted with H2O and extracted several times with Et2O, the washed and dried extract filtered and evaporated, the pigment resin distributed between 50 cc. MeOH and 70 cc. petr. ether (b. $30-60^{\circ}$), filtered from precipitated I, the epiphase extracted with 50 cc. 90% MeOH, the combined MeOH exts. evaporated, taken

up in MeOH and centrifuged at 3500 r.p.m. with addition of petr. ether, the precipitate again precipitated by centrifugation from MeOH and petr. ether, the powdery

product taken up in C6H6, filtered and the filtrate evaporated in vacuo, the residue dried at 40° in vacuo, combined with precipitated I and extracted with boiling C6H14, the insol. residue crystallized from MeOH, the crude pigment (57.7 mg., m. 175.0-7.5°) recrystd. from MeOH, the coppery-shining prisms (38.9 g., m. 180.5-1.5°) recrystd. slowly from C6H6 and C6H12 gave 32.0 g. reddish granular I, C40H66O4, m. 183.5-4.0°, λ 501.5, 469, 442 m μ (in CS2); 48.5, 455, 428.5 m μ (ϵ 132,300, 138,600, 91,700, in C6H6). I is isomeric with violaxanthin (II), λ 483, 453.5, 428 m μ (ϵ 128,400, 134,400, 88,500, in C6H6) and trollixanthin (III), λ 482, 454, 427 m μ [ϵ 121,800, 127,700, 84,400, in C6H6, trans form (IIIa)]. I differs from II which gives a very stable dark blue salt with 20% HCl. On shaking in Et2O with 25% (or stronger) HCl pure I gives a faint pos. blue coloration indicative of the presence of an epoxy grouping or its rearrangement product. The combined mother liquors from crystallization of I taken up in 50

CHCl3, the red solution treated with $5~{\rm cc.}~0.012N$ HCl in CHCl3, after 90 sec. the green solution shaken with excess aqueous NaHCO3, the bright red mixture washed

with H2O, filtered through an adsorbent cotton column, and the filtrate evaporated in vacuo gave a residue, λ 459.5, 435 m μ (in C6H6). The residue in C6H6 chromatographed over a 4:1 CaCO3-Celite column (7.4 + 22 cm.), developed with 1 l. C6H6-petr. ether and 550 cc. C6H6, the egg-yellow zone eluted with Et2O-MeOH, the eluate evaporated and the pigment taken up in 2 cc. C6H6, the solution treated with excess petr. ether and filtered, the yellow substance recrystd. from MeOH at -15° , and the yellow microcryst. product twice recrystd. from MeOH at -20° and again from MeOH at 0° gave tarachrome (IV), m. 154-64°, λ , 460, 434 m μ (in C6H6); 478, 449 m μ (in CS2). Further purification by chromatography on 4:1 ZnCO3-Celite from C6H6 with 15% Me2CO3 by elution of the egg-yellow zone with Et2O-MeOH and crystallization

CC.

MeOH yielded 3 mg., m. 162-8°, λ 460, 431.5, 407.5 m μ (ϵ 118,000, 119,400, 74,900), indicative of a sterically nonhindered all-trans polyene system, and practically congruent with the curves of trollichrome (V), flavoxanthin, and chrysanthemaxanthin. The chromatograms gave no evidence of an isomeric mixture such as occurs in the acid rearrangement of xanthophyll epoxide (VI). I liberates 3 moles CH4 in Zerevitinov active-H determination and consumes 10.7 moles H in hydrogenolysis.

I is regarded as an hydroxylated VI of which IV is the furanoid rearrangement product. Pure I (16.6 mg.) in 13 cc. CHCl3 treated with 0.012N HCl in CHCl3, shaken 90 sec. later with excess NaHCO3 solution, the orange solution worked up to a resin, taken up in Et2O and evaporated (N atmospheric),

and the crystalline residue recrystd. from C6H6 and MeOH gave fine yellow leaflets of IV, m. $162-8^{\circ}$, C40H56O4. Various specimens of previously isolated III, m. $143-5^{\circ}$, $155-6^{\circ}$, and 199° , were reexamd. to check their nonidentity with pure I, since all were rearranged to give the same V, m. 206° . These various forms consist of IIIa, m. 199° , λ 482, 454, 427 m μ (ϵ 121,800, 127,700, 84,400, c 1.07 + 10-5 m., in C6H6), cis-III (IIIb), m. $143-5^{\circ}$, λ 481, 456, 430 m μ (ϵ 50,900, 74,000, 64,000, c 1.182 + 10-5, in C6H6), and a difficultly separated mixture of IIIa and IIIb. All attempts to invert the cis form to the all-trans form gave only unchanged IIIb, V, or decomposition products. The occurrence of IIIb in some specimens of Trollius europaeus (mountain globe flower) and of IIIa in others may depend on the time of harvesting (cf. Zechmeister and Schroeder, C.A. 37, 11529).

IT 117885-38-8

RN

(Derived from data in the 6th Collective Formula Index (1957-1961)) $117885 \hbox{--} 38 \hbox{--} 8$ CAPLUS

CN 1H-Pyrano[3,4-c]pyridinium, 5-ethenyl-3,4-dihydro-7-methyl-1-oxo-, iodide (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH} = \text{CH}_2 \\ \\ \text{O} \\ \\ \text{O} \end{array}$$

• I-

L6 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1946:37331 CAPLUS

DOCUMENT NUMBER: 40:37331
ORIGINAL REFERENCE NO.: 40:7213b-e

TITLE: Alkaloids of Gentiana kirilowi. Structure of

gentianine

AUTHOR(S): Proskurnina, N. F.

SOURCE: Zhurnal Obshchei Khimii (1944), 14, 1148-52

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB Extraction of ground Gentiana kirilowi with dichloroethane in the presence of 10% NH4OH, followed by extraction of the extract with 10% H2SO4, treatment of the

acid extract with excess NH3, and crystallization from ${\tt Et20}$ gave 0.2% crude alkaloid

mass, which, on crystallization from EtOH, gave 0.1% gentianine, m. $79-80^\circ$; HCl salt, m. $171-2^\circ$; H Br salt, m. $177-8^\circ$ (from EtOH); HNO3 salt, m. $238-40^\circ$ (from EtOH); oxalate, m. $152-3^\circ$ (from EtOH); methiodide, m. $190-1^\circ$ (from EtOH). The empirical formula of the alkaloid is C10H9NO2. Hydrogenation over Pt in HCl solution gave dihydrogentianine, m. $75-6^\circ$ (from EtOH), while treatment of the alkaloid with alc. NaOH yielded a precipitate of Na salt of gentianinic acid,

 $132-4^\circ$; the acid is readily transformed into gentianine-HCl on standing in HCl solution, thus indicating the probability of a lactone structure. Oxidation of the alkaloid with KMnO4 in Me2CO yielded an acid, C9H7NO4, m. $260-2^\circ$ (from water), which, on oxidation with alkaline KMnO4, gave an acid, C8H5NO6, m. $265-7^\circ$ (from water in the presence of HCl). Distillation of the alkaloid with Zn dust gave pyridine. The alkaloid

is apparently a 3-vinylpyridine derivative, with a lactone-type bicyclic structure.

IT 117885-38-8P

m.

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Alkaloids of Gentiana kirilowi. Structure of gentianine)

RN 117885-38-8 CAPLUS

CN 1H-Pyrano[3,4-c]pyridinium, 5-ethenyl-3,4-dihydro-7-methyl-1-oxo-, iodide (1:1) (CA INDEX NAME)

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